

Endosulfan sulfate

1031-07-8 | DTXSID3037541

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: $1.23\text{e-}11$ cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: $1.99\text{e-}01$

Confidence level: $7.36\text{e-}01$

Nearest Neighbors from the Training Set

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Cycloate

Measured: $3.54\text{e-}11$

Predicted: $2.98\text{e-}11$

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1-Nitro-2-methylnaphthalene

Measured: $8.00\text{e-}12$

Predicted: $3.49\text{e-}11$

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EPTC

Measured: $3.18\text{e-}11$

Predicted: $2.83\text{e-}11$

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p-Nitroanisole

Measured: $2.46\text{e-}12$

Predicted: $1.65\text{e-}11$

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Isoproturon

Measured: $1.20\text{e-}11$

Predicted: $3.23\text{e-}11$